Optimality of the Neighbor Joining Algorithm and Faces of the Balanced Minimum Evolution Polytope

David C. Haws[1], Terrell L. Hodge[2], and Ruriko Yoshida[1]

[1] University of Kentucky, Lexington, KY, 40502-00227
[2] Western Michigan University, Kalamazoo, MI, 49008-5248

Abstract. Balanced minimum evolution (BME) is a statistically consistent distance-based method to reconstruct a phylogenetic tree from an alignment of molecular data. In 2000, Pauplin showed that the BME method is equivalent to optimizing a linear functional over the BME polytope, the convex hull of the BME vectors obtained from Pauplin's formula applied to all binary trees. The BME method is related to the Neighbor Joining (NJ) algorithm, now known to be a greedy optimization of the BME principle. Further, the NJ and BME algorithms have been studied previously to understand when the NJ Algorithm returns a BME tree for small numbers of taxa. In this paper we aim to elucidate the structure of the BME polytope and strengthen knowledge of the connection between the BME method and NJ Algorithm. We first prove that any subtree-prune-regraft move from a binary tree to another binary tree corresponds to an edge of the BME polytope. Moreover, we describe an entire family of faces parametrized by disjoint clades. We show that these *clade-faces* are smaller dimensional BME polytopes themselves. Finally, we show that for any order of joining nodes to form a tree, there exists an associated distance matrix (i.e., dissimilarity map) for which the NJ Algorithm returns the BME tree. More strongly, we show that the BME cone and every NJ cone associated to a tree T have an intersection of positive measure.

Keywords: Phylogentic Analysis, Balanced Minimum Evolution, Neighbor Joining, Polyhedral Geometry, Combinatorics.

1 Introduction

Current efforts to reconstruct the tree of life for different organisms demand the inference of phylogenies from thousands of DNA sequences (see http://tolweb.org/tree/ [1] and [7] for more details). Large scale projects include the investigation of the tree of life for flies, by researchers at North Carolina State University (`http://www.inhs.illinois.edu/research/FLYTREE/`), the tree of life for fungi, at Duke University (`http://aftol.org`/), and at the University of Kentucky, the tree of life for the insect order Hymenoptera (`http://www.hymatol.org/`).

The most established approach to tree reconstruction is the maximum likelihood (ML) method. In this method, evolution is described in terms of a discrete-state continuous-time Markov process on a phylogenetic tree. Unfortunately, an exhaustive search for the ML phylogenetic tree is computationally prohibitive for large data sets [20]. However, one can efficiently compute a pairwise distance, a distance between a pair of leaves, using the ML method. The pairwise distances can then be used, together with a distanced-based tree reconstruction method, to recover the phylogenetic tree that relates the sequences [17], albeit at a loss of accuracy. To date, distance-based methods for phylogeny reconstruction have been seen to be the best hope for accurately building phylogenies on very large sets of taxa such as the data sets for tree of life for Hymenoptera [13, 23]. More precisely, distance-based methods have been shown to be statistically consistent in all settings (such as the long branch attraction) in contrast with parsimony methods [4, 10, 11, 16]. Distance-based methods also have a huge speed advantage over parsimony and likelihood methods, and hence enable the reconstruction of trees on greater numbers of taxa.
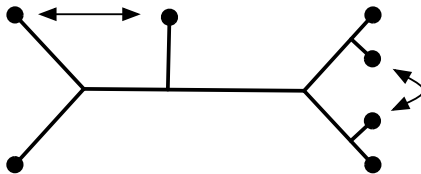
In 2002, Desper and Gascuel introduced a balanced minimum evolution (BME) principle, based on a branch length estimation scheme of Pauplin [19]. The guiding principle of minimum evolution tree reconstruction methods is to return a tree whose total length (sum of branch lengths) is minimal, given an input dissimilarity map. The BME method is a special case of these distance-based methods wherein branch lengths are estimated by a weighted least-squares method (in terms of the input dissimilarity map and the tree in question) that puts more emphasis on shorter distances than longer ones. Each labeled tree topology gives rise to a vector, called herein *the BME vector,* which is obtained from Pauplin's formula.

Implementing, exploring, and better understanding the BME method have been focal points of several recent works. The software `FastME`, developed by Desper and Gascuel, heuristically optimizes the BME principle using nearest-neighbor interchanges (NNI) [12]. In simulations, `FastME` gives superior trees compared to other distance-based methods, including one of biologists' most popular distance-based methods, the Neighbor Joining (NJ) Algorithm, developed by Saitou and Nei [21]. In 2000, Pauplin showed that the BME method is equivalent to optimizing a linear function, the dissimilarity map, over the BME representations of binary trees, given by the BME vectors [19]. Eickmeyer et. al. defined the nth *BME polytope* as the convex hull of the BME vectors for all binary trees on a fixed number n of taxa. Hence the BME method is equivalent to optimizing a linear function, namely, the input dissimilarity map, over a BME polytope. In 2010, Matsen and Cueto [8] studied how the BME method works when the addition of an extra taxon to a data set alters the structure of the optimal phylogenetic tree. They characterized the behavior of the BME phylogenetics on such data sets, using the BME polytopes and the *BME cones*, i.e., the normal cones of the BME polytope.

Eickmeyer et. al. studied the BME polytopes computationally, for unrooted phylogenetic trees with eight or fewer taxa. In addition to this computational study of the BME polytopes, they showed the following general lemma:

Lemma 1 (Lemma 3.1 in [14]). *For any number of taxa n, the vertices of the nth BME polytope are exactly the BME vectors of all unrooted binary trees with n leaves. The BME vector of the star phylogeny lies in the interior of the BME polytope, and all other BME vectors lie on the boundary of the BME polytope.*

In particular, Eickmeyer et. al. studied edges of the BME polytopes computationally. They found that the edge graph of the nth BME polytope is the

Fig. 1. The non-edges on the nth BME polytope for $n = 7$. Two trees will form a non-edge if and only if they are trees that have three cherries, and differ by the pair of leaf exchanges shown in the figure.

complete graph T_2 with the same number (≤ 6) of leaves, there is a dissimilarity map for which T_1 and T_2 are (the only) co-optimal BME trees. However, for $n = 7$, the BME polytope has one combinatorial type of non-edge, i.e., the BME vectors of two bifurcating trees with seven leaves and three cherries (two leaves adjacent to the unique internal node in the tree) fail to be joined by an edge if and only if their trees are related by two leaf exchanges as depicted in Figure 1. This completely characterizes the non-edges for $n = 7$.

Characterizing the edges of the nth BME polytope for $n > 7$ remains an open problem that motivated this work. Understanding the structure of the BME polytope through its edges and faces may help with the development of new optimization strategies to find an optimal BME tree. For example, one such approach could entail employing an edge-walking method over the edges of the BME polytope, since the BME method is a linear programming problem over the BME polytope. However, until now, not much was known about the faces of the BME polytopes besides vertices (which are trivial to characterize).

This paper makes contributions towards understanding both edges and higher-dimensional faces of the BME polytope. First, we prove that any subtree-prune-regraft (SPR) move from a binary tree to another binary tree corresponds to an edge of the BME polytope. This implies that any NNI move from a binary tree to another binary tree corresponds to an edge of the BME polytope. Consequently,

the method implemented in the software `FastME` is an edge-walking method over the edges of the BME polytope using NNI moves. Moreover, we define and describe an entire family of faces of the BME polytope that are parametrized by disjoint clades. We show that these *clade-faces* are smaller dimensional BME polytopes themselves.

The study of related geometric structures, the BME cones, further clarifies the nature of the link between phylogenetic tree reconstruction using the BME criterion and using the Neighbor Joining (NJ) Algorithm. In 2006, Gascuel and Steel showed that the NJ Algorithm, one of the most popular phylogenetic tree reconstruction algorithms, is a greedy algorithm for finding the BME tree associated to a dissimilarity map [18]. The Neighbor Joining Algorithm relies on a particular criterion for iteratively selecting cherries; details on cherry-picking and the NJ Algorithm are recalled later in the paper. In 2008, based on the fact that the selection criterion for cherry-picking is linear in the dissimilarity map [5], Eickmeyer et. al. showed that the NJ Algorithm will pick cherries to merge in a particular order and output a particular tree topology T if and only if the pairwise distances satisfy a system of linear inequalities, whose solution set forms a polyhedral cone in $\mathbb{R}^{\binom{n}{2}}$ [14]. They defined such a cone as an *NJ cone*. In general, the sequence of cherries chosen by the NJ Algorithm is not unique, hence multiple dissimilarity maps will be assigned by the NJ Algorithm to a single fixed tree topology T. The set of all dissimilarity maps for which the NJ Algorithm returns a fixed tree topology T is a union of NJ cones, however this union is not convex in general. Eickmeyer et. al. [14] characterized those dissimilarity maps for which the NJ Algorithm returns the BME tree, by comparing the NJ cones with the BME cones, for eight or fewer taxa.

Yet, before this paper, it was unclear whether, given a tree topology T with an arbitrary number of taxa, and any particular order of picking cherries allowed by the NJ Algorithm, there existed a dissimilarity map such that the NJ Algorithm would return the BME tree T. We prove this in fact is so, despite the fact that greedy algorithms do not generally construct the globally optimal structure for the condition which they locally optimize. Interpreted in terms of phylogenetics, this is particularly important, as it shows that there is no order of picking cherries for which the NJ Algorithm will fail to return the BME tree. Geometrically this means that for any NJ cone associated with the tree topology T and a particular choice of cherry-picking order, there exists a non-empty intersection with the BME cone associated with T. Consequently, given any tree topology T, there exists a dissimilarity map such that NJ and BME both return the tree topology T. More strongly, we show that the BME cone and every NJ cone associated to a tree T have an intersection of positive measure.

This paper is organized as follows: Definitions and notation are covered in Section 2. Subsection 2.4 treats clade-faces of the BME polytope and contains a useful proposition concerning objective criteria for greedy linear optimization. Section 3 contains the proof that two trees adjacent by an SPR move form an edge of the BME polytope. In Section 4 we present the Cherry Forcing Algorithm and show that it also provides proof for the existence of clade-faces. Finally,

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using the Cherry Forcing Algorithm, in Section 5 we prove that every NJ cone associated with a tree T has a non-empty intersection of positive measure with the BME cone associated with T. That is, given a tree T and a sequence of cherries chosen by the NJ Algorithm, there is a dissimilarity map such that NJ and BME return T. We finish with a discussion in Section 6.

2 Notation, Definitions and Further Preliminaries

2.1 Phylogenetic X-trees, Cherries, and Clades

Let X be a set of leaves, which we also may call taxa; when $|X| = n$, we will often conveniently identify X with $\{1, 2, \ldots n\}$. A *dissimilarity map* (or *distance matrix*) is a function $d : X \times X \to \mathbb{R}$ with $d(x, x) = 0$ and $d(x, y) = d(y, x)$ for all $x, y \in X$. It is convenient to represent a dissimilarity map by a vector $\mathbf{d} \in \mathbb{R}^{\binom{n}{2}}$. In general, we index entries of any $\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$ by pairs $\{i, j\} \subset X$ with $i < j$ in lexicographic order, i.e. $\mathbf{c} = (c_{12}, c_{13}, \ldots, c_{1n}, c_{23}, \ldots, c_{2,n}, \ldots, c_{n-1,n}) \in \mathbb{R}^{\binom{n}{2}}$. We may also index a set of vectors in $\mathbb{R}^{\binom{n}{2}}$ by superscript when necessary, e.g., $\mathbf{c}^k \in \mathbb{R}^{\binom{n}{2}}$ with $ijth$ coordinate c_{ij}^k. Define $\mathbf{e}_{ij} \in \mathbb{R}^{\binom{n}{2}}$ to be the vector with 1 at the ijth entry and 0 else. Let $\mathbb{R}_+^{\binom{n}{2}} = \{\mathbf{x} \in \mathbb{R}^{\binom{n}{2}} \mid x_{ij} \geq 0 \text{ for all } 1 \leq i < j \leq n\}$.

Mathematically, a *tree* is an undirected graph in which any two vertices are connected by exactly one simple path; the number of edges incident to any vertex (i.e., node) x of the tree is the degree $deg(x)$ of x. If the graph consists of more than a single vertex, a node x with $deg(x) = 1$ is *external*, or a *leaf*; all other nodes are *internal*. A *phylogenetic X-tree* is a tree T with set of leaves X and all internal vertices of degree at least three. Those for which the internal vertices are all of degree three are here called *binary X-trees* (or just *binary trees*, when the context is clear). For $n = |X| \geq 3$ the binary X-trees are necessarily unrooted trees, and for $n \geq 4$, correspond in phylogenetics to unrooted cladograms with no polytomy. Let $\mathcal{T}_n$ be the set of all binary trees with n leaves; we will assume throughout $n \geq 3$. Write $E(T)$ for the set of edges (i.e., branches) of $T \in \mathcal{T}_n$. An edge $e \in E(T)$ is *internal* (resp., *external*) if it does not (resp., does) touch a leaf. A *cherry* of $T \in \mathcal{T}_n$ is a pair of leaves $\{i, j\}$ such that the path between them consists of just two (necessarily external) edges. An *edge-weighting* (or *branch length assignment*) ω of T is a function $\omega : E(T) \to \mathbb{R}$ with $\omega(e) \geq 0$ for every $e \in E(T)$. Given an edge weighting ω, define the *total tree length* $\omega(T) := \sum_{e \in E(T)} \omega(e)$.

An *X-split* is a partition $A \mid B$ of X into two subsets (blocks) $A, B \subset X$. Any edge $e \in E(T)$ of $T \in \mathcal{T}_n$ induces an X-split $A_1 \mid A_2$ by deleting e from T and letting A_i be the subset of leaves associated to the resulting connected component C_i, $i = 1, 2$, of T. Conversely any X-split $A_1 \mid A_2$ corresponds to the edge that when deleted gives the split. When $e \in E(T)$ is internal, we will call C_i a *clade*, and A_i the *support* $\mathrm{supp}(C_i)$ of C_i. When the context is clear, we may identify a clade C with its support $\mathrm{supp}(C)$. By allowing for the case of choosing no edge e, that is, the trivial X-split $\emptyset \mid X$, we obtain T itself as a clade.

Further, we simply say a clade C is in $\mathcal{T}_n$ (and write $C \in \mathcal{T}_n$) if C is a clade for some tree in $\mathcal{T}_n$.

For example, leaves $\{1, 2\}$ define a clade of T_1 of Figure 3(a) whereas $\{2, 3\}$ is not a clade of T_1 since there is no subgraph containing $\{2, 3\}$ attainable by removing an internal edge of T_1. We say two clades $C_1, C_2 \in \mathcal{T}_n$ are *disjoint* if $\mathrm{supp}(C_1) \cap \mathrm{supp}(C_2) = \emptyset$. If C_1, C_2 are disjoint clades both contained in a tree $T \in \mathcal{T}_n$, then we define the *distance between clades* $d_T(C_1, C_2)$ as the number of edges between clades C_1 and C_2 in T.

Finally, given $T \in \mathcal{T}_n$, let $\Sigma(T)$ denote the set of X-splits defined by removal of an edge of T. It is well-known [6] that phylogenetic X-trees $T_1, T_2 \in \mathcal{T}_n$ are determined up to equivalence (as graphs) exactly when $\Sigma(T_1) = \Sigma(T_2)$. If $\omega : E(T) \to \mathbb{R}$ is an edge-weighting, and $A \,|\, B$ is a split in $\Sigma(T)$ with corresponding edge $e \in E(T)$, set $\omega(A \,|\, B) := \omega(e)$. A distance matrix $\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$ is called an *additive metric* or *tree metric* if $\mathbf{c}$ is a metric, and there exists a tree $T \in \mathcal{T}_n$ and an edge-weighting ω on T s.t.

(a) $\omega(e) > 0$ for all $e \in E(T)$.
(b) For every pair of leaves $\{i, j\}$, $c_{ij} = \sum_e \omega(e)$, summing over edges e along the path from leaf i to leaf j.

Clearly, given $T \in \mathcal{T}_n$ and an edge-weighting ω on T, setting $D_{T,\omega}(i, j) = \sum_e \omega(e)$, for the sum as in (b) above, yields a tree metric $D_{T,\omega} \in \mathbb{R}_+^{\binom{n}{2}}$. Given a tree $T \in \mathcal{T}_n$ and any split $A \,|\, B$ in T, where $A, B \subseteq \{1, 2, \ldots, n\}$, the *split metric* is defined as $D^{A\,|\,B} = (d_{ij}^{A\,|\,B})$ where $d_{ij}^{A\,|\,B} = 1$ if $i \neq j$ and $|\{i, j\} \cap A| = 1$, and $d_{ij}^{A\,|\,B} = 0$ else. Thus each split $A \,|\, B$ defines a metric $D^{A\,|\,B}$ from T for which all branch lengths equal to zero, except for the branch e corresponding to $A \,|\, B$. For any edge-weighting ω of T, the split metrics for T and the natural tree metric $D_{T,\omega}$ are related as below (see, e.g., [2]):
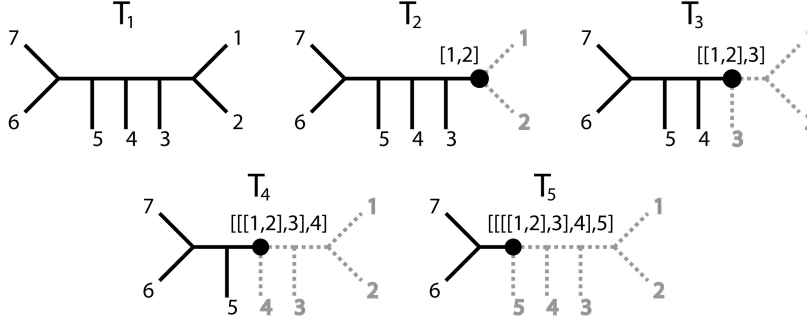
$$D_{T,\omega} = \sum_{A\,|\,B \in \Sigma(T)} \omega(A \,|\, B) D^{A\,|\,B}. \tag{1}$$

2.2 Amalgamation of Cherries

The *amalgamation* of $T \in \mathcal{T}_n$ by cherry $\{i, j\}$ is the subtree $\widetilde{T}$ on $n - 1$ leaves obtained by amalgamating the vertices in cherry $\{i, j\}$ to their common internal parent node. In the more formal mathematical language of relations on the set of leaves $X = \{x_1, \ldots, x_n\}$, the amalgamation of a cherry $\{x_i, x_j\} \in X \times X$ to its common internal parent node $v_{i,j}$ corresponds to a two-step merge obtained (without loss of generality) by first merging the nodes $x_i, v_{i,j}$ to a new (internal) node $v'_{i,j}$, and then merging $x_j, v'_{i,j}$ to a new (external) node $[x_i, x_j]$, resulting in the new tree $\widetilde{T}$ on the leaf set $\widetilde{X} = X - \{x_i, x_j\} \cup \{[x_i, x_j]\}$.

For example, in Figure 2, amalgamating cherry $\{1, 2\}$ of T_1 gives T_2 with the new leaf labeled $[1, 2]$. Next, amalgamating cherry $\{[1, 2], 3\}$ in T_2 produces T_3. If T' is obtained from T by successive amalgamations of cherries (including the

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possibility that no cherries are amalgamated, so $T' = T$), then any leaf i' of T' is either present in T as a single leaf, or the result of the amalgamation of leaves $i_1, \ldots, i_t$ of T. Hence, leaf i' of T' induces the clade C of T with $\mathrm{supp}(C) = \{i'\}$, in the first case, or $\mathrm{supp}(C) = \{i_1, \ldots, i_t\}$, in the second case. For example, leaf $[[[1, 2], 3, 4]]$ of T_4 in Figure 2 defines a clade in T_1 given by the leaves 1,2,3, and 4 of T_1. We will call the clade of T obtained from any leaf i' of T' the *subgraph of T given by i'*.

Fig. 2. Cherry $\{1, 2\}$ of tree T_1 is amalgamated yielding tree T_2, where the new leaf is labeled $[1, 2]$. Cherry $\{[1, 2], 3\}$ of T_2 is amalgamated yielding tree T_3, where the new leaf is labeled $[[1, 2], 3]$. Similarly, the leaves $\{[[1, 2], 3], 4\}$, $\{[[[1, 2], 3], 4], 5\}$ are amalgamated in trees T_3 and T_4, respectively.

2.3 Balanced Minimum Evolution: Method, Vectors, and Polytopes

For a phylogenetic X-tree $T \in \mathcal{T}_n$ and a dissimilarity map $\mathbf{d} \in \mathbb{R}_+^{\binom{n}{2}}$, there are different biologically relevant methods to assign branch lengths (i.e., an edge-weighting) to T; in this context, the entry $d_{i,j}$ of $\mathbf{d}$ is most often regarded as the distance between any pair of taxa i and j. The balanced minimum evolution (BME) method employs a weighted least squares approach for assigning branch lengths $l : E(T) \to \mathbb{R}^+$ given the dissimilarity map $\mathbf{d}$. Defined by Pauplin [19], the definition of the edge-weights $l(e)$ (i.e., [13, Equations (2), (3), equiv., (7), (8)]) utilizes average distances between clades whence consequently the $l(e)$ are, moreover, linear in the input dissimilarity map $\mathbf{d}$ (e.g., see Equation (1) in [13]). However, for the BME method, the calculation of the total tree length $l(T) = \sum_{e \in E(T)} l(e)$ can be easily stated and quickly computed without resorting to computing individual branch lengths $l(e)$, by the means we now describe. For any pair $\{i, j\}$ of leaves of T, define $y_{ij}^T := \#\{$ edges between leaves i and $j \}$, the topological distance between i and j. Set $w_{ij}^T := 2^{1-y_{ij}^T}$, so $\mathbf{w}^T := (w_{12}^T, w_{13}^T, \ldots, w_{n-1,n}^T) \in \mathbb{R}^{\binom{n}{2}}$ is a vector depending only on the topology

of T. Pauplin's [19] formula for the *balanced tree length estimation* (or *estimated BME length*) $l(T)$ is given by

$$l(T) = \sum_{i,j:i<j} w_{i,j}^T d_{i,j} = \mathbf{w}^T \cdot \mathbf{d}. \tag{2}$$

When necessary for clarity, we will also indicate the dependence on $\mathbf{d}$ of the estimated BME length $\mathbf{w}^T \cdot \mathbf{d}$ by writing $l(T, \mathbf{d})$. Since $\mathbf{w}^T$ depends only on the topology of T, but determines $l(T, \mathbf{d})$ given any input dissimilarity map $\mathbf{d} \in \mathbb{R}_+^{\binom{n}{2}}$, we call $\mathbf{w}^T$ the *BME vector for T*.

In [25], the authors in fact defined terms $w_{i,j}^T$ for any phylogenetic X-tree T (not necessarily binary) in terms of certain cyclic permutations of ("circular orderings") of X that respect the structure of T as measured through its set of splits $\Sigma(T)$. In the case of edge-weighted binary X-trees, one recovers the expression for $w_{i,j}^T$ in the BME vector and Pauplin's formula. [25] used this perspective to establish the consistency of the balanced tree length estimation. That is, if $T \in \mathcal{T}_n$ has branch lengths ω and one takes $\mathbf{d} = D_{T,\omega}$ in Equation 2, one obtains $l(T) = \omega(T)$.

The *BME method* for phylogenetic tree reconstruction (or *BME principle*) can be succinctly stated: find a $T \in \mathcal{T}_n$ such that Equation 2 is minimized, given the dissimilarity map $\mathbf{d} \in \mathbb{R}^{\binom{n}{2}}$.

Note that one can efficiently compute the input for the BME method, i.e., pairwise distances $d(i,j)$, from any given sequence alignment using the maximum likelihood estimators (MLEs) under an evolutionary model. The BME method for tree reconstruction was shown to be consistent in [13].

We recall some necessary definition from polyhedral geometry [22]. The *convex hull* of $\{\mathbf{a}_1, \ldots, \mathbf{a}_m\} \subset \mathbb{R}^n$ is defined as

$$\text{conv}\{\mathbf{a}_1, \ldots, \mathbf{a}_m\} := \left\{ \mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} = \sum_{i=1}^m \lambda_i \mathbf{a}_i, \ \sum_{i=1}^m \lambda_i = 1, \ \lambda_i \geq 0 \right\}.$$

A *polytope* $\mathcal{P}$ is the convex hull of finitely many points. We say $F \subseteq P$ is a *face* of the polytope $\mathcal{P}$ if there exists a vector $\mathbf{c}$ such that $F = \text{argmax}_{\mathbf{x} \in \mathcal{P}} \mathbf{c} \cdot \mathbf{x}$. Every face F of $\mathcal{P}$ is also a polytope. If the dimension of $\mathcal{P}$ is d, a face F is a *facet* if it is of dimension $d-1$. A face is an *edge* if it is of dimension two. Denote the vertex set of a polytope $\mathcal{P}$ by $\text{vert}(\mathcal{P})$, where a vertex of a d-dimensional polytope is the intersection point of d or more edges, faces or facets.
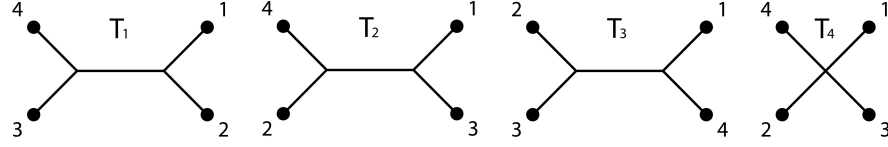
With the background on BME above in hand, we now recall the definition of the central object of study in this paper, the BME polytope, as it arises from the BME vectors.

Definition 1 (BME polytope). *The balanced minimum evolution (BME) polytope $\mathcal{P}_n$ on n leaves is defined as*
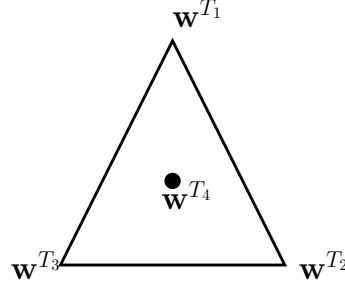
$$\mathcal{P}_n := \text{conv}\left\{ \mathbf{w}^T \mid T \in \mathcal{T}_n \right\}.$$

If F is a face of $\mathcal{P}_n$, then its vertex set is given by $\mathrm{vert}(F) = \{\mathbf{w}^{T_1}, \ldots, \mathbf{w}^{T_m} \mid \mathbf{w}^{T_i} \in F\}$, which we may identify with the set of trees $\{T_1, \ldots, T_m\}$. With this definition we can see that minimizing Equation 2 is equivalent to minimizing the linear objective $\mathbf{d} \in \mathbb{R}^{\binom{n}{2}}$ over $\mathcal{P}_n$. Using Day's results it can be shown that choosing a minimizing tree for (2) from among the $(2n-5)!!$ unrooted binary trees is an NP-hard problem [9, 14]. Thus it is NP-hard to optimize linearly over $\mathcal{P}_n$ [14].

(a) For $|X| = 4$, there are the 3 binary trees and the star-shaped tree.

(b) BME polytope on four taxa.

Fig. 3. All X-trees on four taxa and the BME polytope $\mathcal{P}_4$

Example 1 ([14]). For $n = 4$, there are the 3 binary trees and the star-shaped tree as in Figure 3(a). For this case the BME polytope is the convex hull of the vectors:

$$\mathbf{w}^{T_1} = \left(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right), \quad \mathbf{w}^{T_2} = \left(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right),$$

$$\mathbf{w}^{T_3} = \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right), \quad \mathbf{w}^{T_4} = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$$

Thus the BME polytope $\mathcal{P}_n$ for $n = 4$ is a triangle in $\mathbb{R}^6$. Note that the star-shaped tree is in the interior of $\mathcal{P}_n$.

Remark 1 ([14]). The nth BME polytope $\mathcal{P}_n$ lies in $\mathbb{R}^{\binom{n}{2}}$ and has dimension $\binom{n}{2} - n$.

2.4   Clade Faces

With minor modifications of the proof of BME consistency in [13] we will show that any collection of disjoint clades defines a face of the BME polytope. This will also be proved independently and constructively in Section 5 using the Cherry Forcing Algorithm.

Lemma 2. *Let $C_1, \ldots, C_p \in \mathcal{T}_n$ be a pairwise disjoint collection of clades. There exists a $\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$ such that $\underset{T \in \mathcal{T}_n}{\operatorname{argmax}} \, \mathbf{w}^T \cdot \mathbf{c} = \{\, T \in \mathcal{T}_n \mid C_1, \ldots, C_p \in T \,\}$.*

See the appendix for a proof of Lemma 2.

Lemma 2 proves that every disjoint set of clades corresponds to a face of $\mathcal{P}_n$ which we define as follows: Given a set of disjoint clades $\{C_1, \ldots, C_p \mid C_i \in \mathcal{T}_n, \, \forall \, 1 \leq i \leq p\}$, we define a *clade-face* of the BME polytope $\mathcal{P}_n$ by $F_{C_1, \ldots, C_p} := \{\, T \in \mathcal{T}_n \mid C_1, \ldots, C_p \in T \,\}$. Moreover, the face $F_{C_1, \ldots, C_p}$ is the image of an affine transformation of the BME polytope $\mathcal{P}_l$, where $l := n - \sum_{i=1}^{p}(|C_i| - 1)$. This follows since every tree in $F_{C_1, \ldots, C_p}$ can be constructed by starting with a binary tree on l leaves and attaching the clades $\{C_1, \ldots, C_p\}$ to p of the l leaves.

Looking ahead to Section 3, one can see that the three trees corresponding to a nearest neighbor interchange (explained therein) form a clade-face, as an immediate consequence of Lemma 2. This suggests that NNI and SPR moves yield edges of the BME polytope $\mathcal{P}_n$, but this fact will require additional proof. Leading into this, we provide a proposition which holds for any polytope in general, and will be key to our further arguments. Roughly speaking it states that if the entries of $\mathbf{c}_1$ are significantly larger than the entries of $\mathbf{c}_2$, then when linearly optimizing $\mathbf{c}_1 + \mathbf{c}_2$ over a polytope $\mathcal{P}$ then $\mathbf{c}_1$ must be maximized foremost.

Proposition 1. *Let $\mathcal{P} \subseteq \mathbb{R}^m$ be a polytope and $\mathbf{c}_1, \mathbf{c}_2 \in \mathbb{R}^m$. If*

$$\min_{\substack{\mathbf{x}, \mathbf{y} \in \operatorname{vert}(\mathcal{P}) \\ \mathbf{x} \in \operatorname{argmax}_{\mathbf{z} \in \mathcal{P}} \mathbf{c}_1 \cdot \mathbf{z} \\ \mathbf{c}_1 \cdot \mathbf{x} \neq \mathbf{c}_1 \cdot \mathbf{y}}} \mathbf{c}_1 \cdot \mathbf{x} - \mathbf{c}_1 \cdot \mathbf{y} > \max_{\mathbf{x}, \mathbf{y} \in \operatorname{vert}(\mathcal{P})} |\mathbf{c}_2 \cdot \mathbf{x} - \mathbf{c}_2 \cdot \mathbf{y}| \qquad (3)$$

then

$$\operatorname*{argmax}_{\mathbf{z} \in \operatorname{vert}(\mathcal{P})} (\mathbf{c}_1 + \mathbf{c}_2) \cdot \mathbf{z} \subseteq \operatorname*{argmax}_{\mathbf{z} \in \operatorname{vert}(\mathcal{P})} \mathbf{c}_1 \cdot \mathbf{z}.$$

See the appendix for a proof of Proposition 1.

Consider two clade-faces $F_{C_1, \ldots, C_k}$ and $F_{C'_1, \ldots, C'_{k'}}$ where $|F_{C_1, \ldots, C_k}| > 1$. Then, $F_{C'_1, \ldots, C'_{k'}} \subseteq F_{C_1, \ldots, C_k}$ if and only if for every $1 \leq i \leq k$, clade C_i is contained in, or equal to, clade C'_j for some $1 \leq j \leq k'$. If $F_{C_1, \ldots, C_k} = \{T\}$, then $F_{C'_1, \ldots, C'_{k'}} \subseteq F_{C_1, \ldots, C_k}$ if $F_{C'_1, \ldots, C'_{k'}} = \{T\}$. We note that this induces a partial order on the clade-faces of $\mathcal{T}_n$, and gives a lattice if one also considers $\mathcal{P}_n$ and the empty set as clade-faces.

3 SPR Adjacency Implies BME Adjacency

A *subtree-prune-regraft* (SPR) move on a tree $T \in \mathcal{T}_n$ is determined by choosing a clade of C of T, pruning it from T, and amalgamating the two internal edges originally connecting C to T to one edge. Finally an internal edge of T is chosen, a node is inserted, and C is attached to this node. For an example, see Figure 4. Thus, T is changed to another binary tree on n leaves and we say the two trees are adjacent by an SPR move.

A nearest neighbor interchange (NNI) move on a tree $T \in \mathcal{T}_n$ is determined by choosing an internal edge $e \in E(T)$, , and rearranging the four subgraphs (clades) that e induces. It is not difficult to see then that an NNI move is also an SPR move. The following lemma is an application of Proposition 1 applied to a face of the BME polytope, and two clades contained in the face.

Lemma 3. *Let F be a face of the BME polytope $\mathcal{P}_n$, where C_1, C_2 are disjoint clades with $C_1, C_2 \in T$, $\forall T \in \mathrm{vert}(F)$. There exists an objective $\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$ such that*

$$\operatorname*{argmax}_{T \in \mathcal{T}_n} \mathbf{w}^T \cdot \mathbf{c} = \{\, T \in \mathrm{vert}(F) \mid d_T(C_1, C_2) \geq d_{T'}(C_1, C_2),\ \forall T' \in \mathrm{vert}(F) \,\}.$$

Similarly there exists an objective $\mathbf{d} \in \mathbb{R}^{\binom{n}{2}}$ such that

$$\operatorname*{argmax}_{T \in \mathcal{T}_n} \mathbf{w}^T \cdot \mathbf{d} = \{\, T \in \mathrm{vert}(F) \mid d_T(C_1, C_2) \leq d_{T'}(C_1, C_2),\ \forall T' \in \mathrm{vert}(F) \,\}.$$
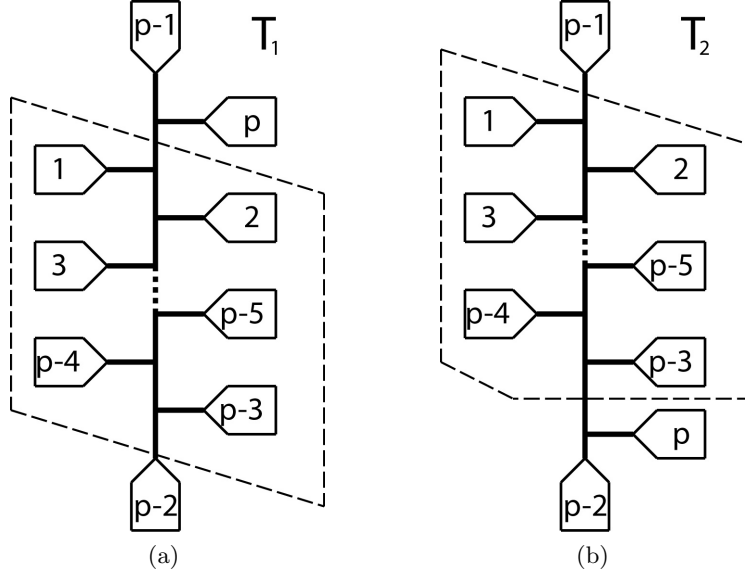
For a proof of Lemma 3 see the appendix.

Corollary 1. *Every NNI move corresponds to an edge of the BME polytope.*

Proof. Simply take the objective $\mathbf{c}$ given by Lemma 2 which yields the face of the three trees corresponding to an NNI, then add the extra criteria that either two of the clades are as close or as far as possible, and apply Lemma 3.

$\square$

We now present our result that any pair of two trees adjacent by an SPR move yields an edge of the BME polytope.

Theorem 1. *If $T_1, T_2 \in \mathcal{T}_n$ are adjacent by an SPR move, then there exists $\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$ such that $\mathbf{w}^{T_1} \cdot \mathbf{c} = \mathbf{w}^{T_2} \cdot \mathbf{c} > \mathbf{w}^T \cdot \mathbf{c}$ for all $T \in \mathcal{T}_n \backslash \{T_1, T_2\}$.*

Proof. Let $T_1, T_2 \in \mathcal{T}_n$ be adjacent by an SPR move. Any such move can be described by Figure 4, where $C_1, \ldots, C_p$ (labeled $1, \ldots, p$ in Figure 4) are clades common to T_1 and T_2 and clade C_p is the subtree that is pruned and regrafted. By Lemma 2 there exists an objective $\mathbf{c}_1 \in \mathbb{R}^{\binom{n}{2}}$ for the clade-face $F_{C_1, \ldots, C_p}$.

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Fig. 4. Here $1, \ldots, p$ are subgraphs (clades). Two trees, T_1 (a) and T_2 (b), adjacent by an SPR move where subgraph p and its connecting edge is the subgraph pruned from T_1 and regrafted between subgraph $(p-2)$ and its internal node.

Note that $T_1, T_2 \in F_{C_1, \ldots, C_p}$, but in general $F_{C_1, \ldots, C_p}$ will contain more trees, hence further restrictions need to be placed on the objective. By repeated use of Lemma 3, and the objective $\mathbf{c}_1$ which defines $F_{C_1, \ldots, C_p}$, there exists an objective $\mathbf{c}_2 \in \mathbb{R}^{\binom{n}{2}}$ such that in this order of importance,

1) the distance between clades C_{p-1} and C_{p-2} is maximized,
2) the distance between clades C_1 and C_2 is minimized,
3) the distance between clades C_2 and C_3 is minimized,
4) the distance between clades C_3 and C_4 is minimized,

   $\vdots$

p-4) the distance between clades C_{p-4} and C_{p-3} is minimized,

for trees in $F_{C_1, \ldots, C_p}$. Since T_1 and T_2 contain the clades $C_1, \ldots, C_p$ and the properties in the previous list are satisfied in the prescribed order, we see that $\{T_1, T_2\} \subset \operatorname{argmax}_{T \in \mathcal{P}_n} \mathbf{w}^T \cdot \mathbf{c}_2$, but the latter may also contain the trees with the clades in the dashed box of Figure 4 inverted vertically.

Select leaves $i \in C_{p-1}$ and $j \in C_1$ such that $d_{T_2}(i, j) \leq d_{T_2}(m, n)$, $\forall (m, n) \in C_{p-1} \times C_1$. Similarly, let $k \in C_{p-2}$ and $l \in C_{p-3}$ such that $d_{T_1}(k, l) \leq d_{T_1}(m, n)$, $\forall (m, n) \in C_{p-2} \times C_{p-3}$.

Let $\mathbf{d} = w_{kl}^{T_1} \mathbf{e}_{ij} + w_{ij}^{T_2} \mathbf{e}_{kl}$. Note that $2w_{ij}^{T_1} = w_{ij}^{T_2}$ and $w_{kl}^{T_1} = 2w_{kl}^{T_2}$. It follows then that $\mathbf{w}^{T_1} \cdot \mathbf{d} = \mathbf{w}^{T_2} \cdot \mathbf{d}$. There exists $\varepsilon > 0$ small enough such that

$$\min_{\substack{\mathbf{x},\mathbf{y}\in\mathrm{vert}(\mathcal{P}) \\ \mathbf{x}\in\mathrm{argmax}_{\mathbf{z}\in\mathcal{P}}\, \mathbf{c}_2\cdot\mathbf{z} \\ \mathbf{c}_2\cdot\mathbf{x}\neq\mathbf{c}_2\cdot\mathbf{y}}} \mathbf{c}_2 \cdot \mathbf{x} - \mathbf{c}_2 \cdot \mathbf{y} > \max_{\mathbf{x},\mathbf{y}\in\mathrm{vert}(\mathcal{P})} |\varepsilon\mathbf{d} \cdot \mathbf{x} - \varepsilon\mathbf{d} \cdot \mathbf{y}|.$$

Therefore Proposition 1 holds and the objective $\varepsilon\mathbf{d}$ optimized over $\mathrm{argmax}_{T\in\mathcal{T}_n}\, \mathbf{w}^T \cdot \mathbf{c}_2$ gives trees such that either clades C_1 and C_{p-1} are as close as possible or C_{p-2} and C_{p-2} are as close as possible. Therefore $\mathrm{argmax}_{T\in\mathcal{T}_n}\, \mathbf{w}^T \cdot (\mathbf{c}_2 + \varepsilon\mathbf{d})$ contains only T_1 and T_2.

$\square$

4 Cherry Forcing Objectives

The following lemma is a sufficient condition for vectors $\mathbf{c}^1, \mathbf{c}^2 \in \mathbb{R}_+^{\binom{n}{2}}$ to satisfy Proposition 1 on the BME polytope $\mathcal{P}_n$.

Lemma 4. *Let $\mathbf{c}^1, \mathbf{c}^2 \in \mathbb{R}_+^{\binom{n}{2}}$ where for a fixed $K > 0$, $\mathbf{c}_{ij}^1 = K$ for all $\{i,j\} \in \mathrm{supp}(\mathbf{c}^1)$. If*

$$\frac{K}{2^{n-2}} > \frac{1}{2}\mathbf{c}^2 \cdot (1, 1, \ldots, 1) \tag{4}$$

then

$$\mathrm{argmax}_{T\in\mathcal{P}_n} (\mathbf{c}^1 + \mathbf{c}^2) \cdot \mathbf{w}^T \subseteq \mathrm{argmax}_{T\in\mathcal{P}_n} \mathbf{c}^1 \cdot \mathbf{w}^T.$$

See the appendix for a proof of Lemma 4. If a triple $(\mathbf{c}^1, \mathbf{c}^2, \mathcal{P}_n)$ satisfies the assumptions and hypothesis of Lemma 4 and Equation 4 then we say it satisfies the *dominance condition*.

Given a clade C in $\mathcal{T}_n$ as input, the idea of the Cherry Forcing Algorithm is to iteratively fill in entries in an objective $\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$ to satisfy the dominance condition given in Equation 4 in such a fashion that respects C. More precisely, under the Cherry Forcing Algorithm, (1) a small part of the topology (e.g. cherry) of C is fixed, and (2) subsequently filled-in entries in $\mathbf{c}$ will be sufficiently small such that no previously fixed structures of C will be broken when maximizing $\mathbf{c} \cdot \mathbf{w}^T$ over $\mathcal{P}_n$. It is proved in Lemma 5 that the sum $\mathbf{c} = \sum_i \mathbf{c}^i$ of the outputs of the Cherry Forcing Algorithm will yield the normal vector to the face of the BME polytope $\mathcal{P}_n$ that consists of all trees that contain C. If C is an entire tree, then the vector $\mathbf{c}$ is in the normal cone of the tree C of $\mathcal{P}_n$. That is, $\mathbf{c} \cdot \mathbf{w}^T$ is maximal only when $C = T$.

Algorithm 1 (Cherry Forcing Algorithm)

1: **input** $\widehat{T} \in \mathcal{T}_n$, *a clade* $\widehat{C}$ *of* $\widehat{T}$.
2: **output** $\mathbf{c}^1, \mathbf{c}^2, \ldots, \mathbf{c}^t \in \mathbb{R}_+^{\binom{n}{2}}$.

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3: *Initialization: Let $T_1 := \widehat{T}$, $K_1 := 1$, $t := 1$, and $\mathbf{c}^i := \mathbf{0} \in \mathbb{R}^{\binom{n}{2}}$.*

4: *repeat*

5:     *Pick a cherry $\{k,l\}$ of T_t, s.t. the subgraphs of $\widehat{T}$ given by k and l are in clade $\widehat{C}$.*

6:     *Let G_k be the nodes of the subgraph of $\widehat{T}$ given by k.*

7:     *Let G_l be the nodes of the subgraph of $\widehat{T}$ given by l.*

8:     *for every pair $\{p,q\} \in G_k \times G_l$ do*

9:       *Let $c^t_{p,q} := \frac{K_t}{\binom{n}{2}}$.*

10:     *Let $K_{t+1} := \frac{K_t}{\binom{n}{2}2^{n-1}}$.*

11:     *Let $t := t + 1$.*

12:     *Let $T_t := T_{t-1}$ where cherry $\{k,l\}$ is amalgamated.*

13: *until T' has a single leaf corresponding to the entire clade $\widehat{C}$ of $\widehat{T}$ or T' is the star tree on three leaves.*

14: *return $\mathbf{c}^1, \mathbf{c}^2, \ldots, \mathbf{c}^t$.*

Lemma 5. *Let $\widehat{T} \in \mathcal{T}_n$ and clade $\widehat{C}$ of $\widehat{T}$ be the input of Algorithm 1 with output $\mathbf{c}^1, \mathbf{c}^2, \ldots, \mathbf{c}^t$. Every triple*

$$\{\mathbf{c}^1, \mathbf{c}^2 + \cdots + \mathbf{c}^t, \mathcal{P}_n\},$$
$$\{\mathbf{c}^2, \mathbf{c}^3 + \cdots + \mathbf{c}^t, \mathcal{P}_n\},$$
$$\{\mathbf{c}^3, \mathbf{c}^4 + \cdots + \mathbf{c}^t, \mathcal{P}_n\},$$
$$\vdots$$
$$\{\mathbf{c}^{t-1}, \mathbf{c}^t, \mathcal{P}_n\}$$

satisfies the dominance condition in Equation 4. Consequently $\operatorname{argmax}_{T \in \mathcal{T}_n}(\sum_{i=1}^t \mathbf{c}^i) \cdot \mathbf{w}^T = \{\, T \in \mathcal{T}_n \mid \widehat{C} \text{ is a clade of } T \,\}.$

A proof of Lemma 5 is provided in the appendix.

Lemma 6. *Let $\widehat{T} \in \mathcal{T}_n$ and clade $\widehat{C}$ of $\widehat{T}$ be the input of Algorithm 1 with output $\mathbf{c}^1, \mathbf{c}^2, \ldots, \mathbf{c}^t$. Then $\operatorname{supp}(\mathbf{c}^i) \cap \operatorname{supp}(\mathbf{c}^j) = \emptyset$ for all $1 \leq i < j \leq t$.*

A proof of Lemma 6 is provided in the appendix.

5   Non-empty Intersection of NJ and BME Cones

The NJ Algorithm, first presented in [21], is a consistent distance-based method to reconstruct a phylogenetic tree. Yet, its biological interpretation and what criteria it optimized have only been established recently. Some initially argued that NJ optimized an ordinary least-squares criteria at each step, while others contended that it did not optimize any criteria. See [18] for a short history of NJ. However in [18], it was shown that in fact, NJ greedily minimizes the BME criteria at every neighbor joining step. In [14] Eickmeyer et. al. characterized

those dissimilarity maps for which the output of the NJ Algorithm is in fact the BME tree, by a comparison of the NJ cones with the BME cones, for eight or fewer taxa.

Given a tree topology $T \in \mathcal{T}_n$ with branch lengths ω, it follows from consistency that NJ and BME will return T given the tree metric $D_{(T,\omega)}$ defined in Section 2.1. That is, $D_{(T,\omega)}$ will lie in at least one NJ cone of T. The order in which NJ picks cherries depends on the dissimilarity map, and the dissimilarity map depends on the branch lengths. Therefore which NJ cone $D_{(T,\omega)}$ lies in is strictly determined by the branch lengths ω. However, if a NJ cone C of T is fixed it is not clear how branch lengths, call it ω', can be assigned to the tree topology of T such that $D_{(T,\omega')}$ is in C. Thus, it is not clear that consistency directly implies that the BME cone and every NJ cone have non-trivial intersection.

Our result is that every NJ cone associated to a tree topology $T \in \mathcal{T}_n$ has an intersection of positive measure with the BME cone. That is, for any NJ cone associated with the particular order to pick cherries and the tree T, there is an intersection of positive measure with the BME cone associated to T, where the BME cone is defined as the set of all dissimilarity maps $\mathbf{d} \in \mathbb{R}^{\binom{n}{2}}$ such that $\mathrm{argmax}_{T' \in \mathcal{T}_n} \mathbf{d} \cdot \mathbf{w}^{T'} \supseteq \{T\}$.

The NJ Algorithm takes as input a dissimilarity map $\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$ and builds a tree $T \in \mathcal{T}_n$ [21]. It involves: 1) picking a cherry $\{i,j\}$, 2) creating a node a joining taxa i and j, 3) computing the distances from other nodes to the new node a, 4) repeating the procedure until the number of leaves n is 3.

The main problem is picking the cherry. A solution, suggested by Saitou and Nei [21] and subsequently modified by Studier and Keppler [26], relies on the Q-criterion in Theorem 2 below.

Theorem 2 (Cherry-picking criterion (Q-criteria) [21, 26]). *Let $\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$ be an additive tree metric for a tree $T \in \mathcal{T}_n$ and define the $n \times n$-matrix $Q_{\mathbf{c}}$ with entries:*

$$Q_{\mathbf{c}}(i,j) = (n-2)c_{i,j} - \sum_{k=1}^{n} c_{i,k} - \sum_{k=1}^{n} c_{k,j} = (n-4)c_{i,j} - \sum_{k \neq j} c_{i,k} - \sum_{k \neq i} c_{k,j}. \quad (5)$$

Then any pair of leaves $\{i^*, j^*\}$, for which $Q_{\mathbf{c}}(i^*, j^*)$ is minimal, is a cherry in the tree T.

If the NJ Algorithm selects taxa $\{k,l\}$ as a cherry, and a is the new node joining $\{k,l\}$ then the new dissimilarity map $\mathbf{c}' \in \mathbb{R}^{\binom{n-1}{2}}$ is defined to be

$$\text{if } i \neq a \neq j \qquad c'_{i,j} = c_{i,j}$$

$$\text{else} \qquad c'_{i,a} = \frac{1}{2}\Big(c_{i,k} + c_{i,l} - c_{k,l}\Big).$$

Lemma 7 (Shifting Lemma [15]). *Let $\mathbf{c}, \mathbf{x} \in \mathbb{R}^{\binom{n}{2}}$ where $\mathbf{x} = (1, 1, \ldots, 1)$. Then the Neighbor Joining Algorithm applied to $\mathbf{c} + k\mathbf{x}$, for any $k \in \mathbb{R}$, returns the same tree as the Neighbor Joining Algorithm applied to $\mathbf{c}$. Moreover, the*

linear ordering of the Q-criteria of $\mathbf{c}$ is the same as the linear ordering of the Q-criteria of $\mathbf{c} + k\mathbf{x}$, i.e. if $Q_{\mathbf{c}}(i_1, j_1) \leq (<) \, Q_{\mathbf{c}}(i_2, j_2)$ then $Q_{\mathbf{c}+k\mathbf{x}}(i_1, j_1) \leq (<) \, Q_{\mathbf{c}+k\mathbf{x}}(i_2, j_2)$.

Lemma 8. *Let $\mathbf{c}^1, \mathbf{c}^2 \in \mathbb{R}_+^{\binom{n}{2}}$ where $|\operatorname{supp}(\mathbf{c}^1)| = 1$, and $(\mathbf{c}^1, \mathbf{c}^2, \mathcal{P})$ satisfies the dominance condition (Equation 4). Further, let $\mathbf{c} = \mathbf{c}^1 + \mathbf{c}^2$, $\{\{p, q\}\} = \operatorname{supp}(\mathbf{c}^1)$, and $Q_{-\mathbf{c}}$ be the Q-criteria calculated from the dissimilarity map $-\mathbf{c}$.*

If $n > 4$, $Q_{-\mathbf{c}}(p, q) < Q_{-\mathbf{c}}(i, j)$ for all $\{i, j\} \neq \{p, q\}$. If $n = 4$, and p, q, r, s are the leaves, then $Q_{-\mathbf{c}}(p, q) = Q_{-\mathbf{c}}(r, s) < Q_{-\mathbf{c}}(i, j)$ where $\{i, j\} \neq \{p, q\}$ and $\{i, j\} \neq \{r, s\}$.

See the appendix for a proof of Lemma 8.

Theorem 3. *Let $\widehat{T} \in \mathcal{T}_n$ be the input for Algorithm 1 with output $\{\mathbf{c}^1, \ldots, \mathbf{c}^t\}$. The Neighbor Joining Algorithm with input $-(\mathbf{c}^1 + \cdots + \mathbf{c}^t)$ returns $\widehat{T}$.*

Proof. We proceed by induction on n. If $n = 3$ we have the star tree and there is nothing to be done. If $n = 4$ then Lemma 5 applies to the output of Algorithm 1 and we are done since NJ will return $\widehat{T}$ by Lemma 8. Consider $n > 4$. Let $\widehat{T} \in \mathcal{T}_n$ be the input for Algorithm 1 with output $\{\mathbf{c}^1, \ldots, \mathbf{c}^t\}$. Define $\mathbf{c} = \mathbf{c}^1 + \cdots + \mathbf{c}^t$. Note also that by Lemma 6, $\operatorname{supp}(\mathbf{c}^1), \ldots, \operatorname{supp}(\mathbf{c}^t)$ are pairwise disjoint. We know Lemma 5 applies and implies by Lemma 4, $\operatorname{argmax}_{T \in \mathcal{T}_n} \mathbf{w}^T \cdot \mathbf{c} = \{\widehat{T}\}$. Let $\{\{p, q\}\} = \operatorname{supp}(\mathbf{c}^1)$ be the first cherry picked in Algorithm 1 and let $Q_{-\mathbf{c}}$ be the Q-criteria of $-\mathbf{c}$. By Lemma 8, $Q_{-\mathbf{c}}(p, q)$ is the minimal element in $Q_{-\mathbf{c}}$. Consider the shifted vector $\mathbf{d} := \mathbf{1} - \binom{n}{2}\mathbf{c} \in \mathbb{R}^{\binom{n}{2}}$, and note that $d_{p,q} = 0$. The Shifting Lemma 7 implies that $Q_{\mathbf{d}}(p, q)$ will be the minimal element in $Q_{\mathbf{d}}$. Thus, the NJ Algorithm will join leaves p and q to the new node a. Consider the new dissimilarity map $\mathbf{d}' \in \mathbb{R}^{\binom{n-1}{2}}$ given by the NJ Algorithm. If $i \neq a$ and $j \neq a$ then $d'_{i,j} = d_{i,j}$. For $i \neq a$, $d'_{i,a} = \frac{1}{2}(d_{i,p} + d_{i,q} - d_{p,q}) = \frac{1}{2}(d_{i,p} + d_{i,q})$, since $d_{p,q} = 0$. Since the cherry $\{p, q\}$ was designated first by Algorithm 1, by construction, for all $i \neq p$ and $i \neq q$, $c^l_{i,p} = c^l_{i,q}$ for all $1 < l \leq t$. This implies $d'_{i,a} = d_{i,p} = d_{i,q}$ for $i \neq a$. Define $\widehat{\mathbf{c}} := \mathbf{1} - \mathbf{d}'$ and $\widehat{\mathbf{c}}^2, \ldots, \widehat{\mathbf{c}}^t \in \mathbb{R}_+^{\binom{n-1}{2}}$ as follows

$$\widehat{c}^l_{i,j} = \begin{cases} \widehat{c}_{i,j} & \text{if } \{i, j\} \in \operatorname{supp}(\mathbf{c}^l) \\ 0 & \text{else} \end{cases}$$

for $2 \leq l \leq t$. Observe that $|\operatorname{supp}(\widehat{\mathbf{c}}^2)| = 1$ since $\widehat{\mathbf{c}}^2$ corresponds to the cherry picked in the amalgamated tree T_2 in Algorithm 1, and p and q have been identified with a. Moreover, every triple $(\widehat{\mathbf{c}}^2, \widehat{\mathbf{c}}^3 + \cdots + \widehat{\mathbf{c}}^t, \mathcal{P}_{n-1})$, $(\widehat{\mathbf{c}}^3, \widehat{\mathbf{c}}^4 + \cdots + \widehat{\mathbf{c}}^t, \mathcal{P}_{n-1})$, ..., $(\widehat{\mathbf{c}}^{t-1}, \widehat{\mathbf{c}}^t, \mathcal{P}_{n-1})$ satisfies the dominance condition of Equation 4. Thus $\operatorname{argmax}_{T \in \mathcal{T}_n} \widehat{\mathbf{c}} \cdot \mathbf{w}^T = \widehat{T}'$ for some $\widehat{T}' \in \mathcal{T}_n$. Since $\widehat{\mathbf{c}}$ is a dissimilarity map on $n - 1$ leaves, the induction hypothesis holds, and NJ returns $\widehat{T}'$. Finally $\widehat{T}'$ is contained in $\widehat{T}$ as a clade, which implies NJ on $-\mathbf{c}$ will return $\widehat{T}$, since $\widehat{T}$ equals the tree $\widehat{T}'$ with leaves i and j connected to leaf a by two different edges.

$\square$

Given a fixed tree topology, Algorithm 1 allows for any choice of neighbor joining pairs (cherries in the NJ Algorithm), and every such choice yields a different NJ cone. Thus, Theorem 3 implies that every NJ cone and BME cone have a non-empty intersection.

Corollary 2. *Every NJ cone C associated to a fixed $T \in \mathcal{T}_n$ has an intersection of positive measure with the BME cone associated to T.*

Proof. Let $T \in \mathcal{T}_n$ be a tree topology and C be a NJ cone associated to T; recall C is also dependent upon an order of picking cherries. Now apply Algorithm 1 with T as the input (as both the tree and clade), choosing cherries in step 5 by the order associated to the NJ cone C, and let $\{\mathbf{c}^1, \ldots, \mathbf{c}^t\}$ be the output. By Theorem 3, the BME and NJ algorithm with input $-\sum_{i=1}^{t} \mathbf{c}^i$ will each return T. Moreover, since the cherries were chosen in step 5 to be consistent with C, we have $-\sum_{i=1}^{t} \mathbf{c}^i \in C$.

Since the BME cone associated to T is convex (as a normal cone of the BME polytope), and $\operatorname{argmin}_{T' \in \mathcal{T}_n}(-\sum_{i=1}^{t} \mathbf{c}^i) = \{T\}$ by Lemma 5, it follows that $-\sum_{i=1}^{t} \mathbf{c}^i$ lies in the interior of the BME cone associated to T.

On the other hand, individual NJ cones are convex (by definition, or see [14]) and the boundary of the intersection of multiple NJ cones associated to the same tree topology corresponds to two or more cherries having equal Q-scores (i.e., Q-criteria entries) at some step in the NJ Algorithm [14]. Lemma 8 implies that the first cherry chosen by the NJ Algorithm will be $\operatorname{supp}(\mathbf{c}^1)$, that is, it has the smallest Q-score with no ties. Moreover, in the proof of Theorem 3 we see that the new dissimilarity map derived from $-\sum_{i=1}^{t} \mathbf{c}^i$ in the NJ Algorithm also satisfies the dominance condition. Hence, Lemma 8 holds again, and there are no ties in the Q-score. Therefore, there will be no ties in the Q-score, except for the case of four taxa. For four taxa, the only ties present are the trivial ones: If S is the set of four taxa ($|S| = 4$) then by definition of the Q-score,

$$Q(p, q) = Q(r, s) \qquad \forall \, \{p, q\} \subseteq S, \, \{r, s\} = S \setminus \{p, q\}.$$

We note that these trivial ties do not correspond to different NJ cones, and hence $-\sum_{i=1}^{t} \mathbf{c}^i$ lies in the interior of C.

In conclusion, we see that $-\sum_{i=1}^{t} \mathbf{c}^i$ lies in the interiors of both the BME cone and the NJ cone C. This implies they have an intersection of positive measure. □

6 Discussion

Mathematically, "closeness" between trees is measured via differing distances (metrics) on tree space $\mathcal{T}_n$, including the popular distance measures $d_{NNI}(T, T')$, $d_{SPR}(T, T')$, and $d_{TBR}(T, T')$ describing the minimum number of nearest neighbor interchange (NNI) (resp., subtree-prune-regrafting (SPR), tree-bisection-regrafting (TBR)) moves needed to transform T to T' for $T, T' \in \mathcal{T}_n$. Each

such metric M yields a notion of adjacency, with $T, T' \in \mathcal{T}_n$ being M adjacent if $d_M(T, T') = 1$. The comparisons of two trees T, T' as NNI, SPR, or TBR adjacent confers useful biological information, including providing the basis for multiple tree reconstruction algorithms [3, 23–25]. For $T, T' \in \mathcal{T}_n$, set $d_{BME}(T, T') = 1$ if $\mathbf{w}^T$ and $\mathbf{w}^{T'}$ are two vertices joined by an edge in the BME polytope $\mathcal{P}_n$. This yields another notion of adjacency in the BME setting.

The point of view of this paper is that knowledge of BME adjacency, and its relationship to NJ adjacency, has likewise the potential to inform our understanding of tree space $\mathcal{T}_n$, and the gene and/or species trees its elements represent. We have explored some relationships between adjacency for $M =$ NNI, SPR, TBR, BME, and NJ. It is well-known that an NNI move is a special case of an SPR move and an SPR move is a special case of a TBR move. In this paper, we have shown that SPR adjacency implies BME adjacency. However it is not known that TBR adjacency implies BME adjacency. We have made some initial explorations in this regard, including using an additional related notion of "circular adjacency" predicated upon the circular orderings employed in [25]. However, having seen no examples to show that TBR adjacency fails to imply BME adjacency, we propose the following conjecture.

Conjecture 1. If $T, T' \in \mathcal{T}_n$, then $d_{TBR}(T, T') = 1$ implies $d_{BME}(T, T') = 1$.

Considering further the potential applications of such adjacency notions in the context of the BME polytopes and BME cones is a topic we hope to explore in a future work.

7   Acknowledgments

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A   Appendix

Proof (Lemma 2).

The proof of the lemma relies almost entirely on the proof in [13] of the consistency of the BME method for phylogenetic tree reconstruction ([13, Theorem 2 and Appendix 3]]). Given $T \in \mathcal{T}_n$ with edge-weighting ω, recall the notation of Section 2.1 and 2.3. Furthermore, from Equations (1) and (2), for any tree $T' \in \mathcal{T}_n$ one can obtain the estimated BME length of T' as a linear function of the metric $D := D_{T,\omega}$ as

$$l(T', D) = \mathbf{w}^{T'} \cdot D = \sum_{A \,|\, B \in \Sigma(T)} \omega(A \,|\, B) l(T', D^{A \,|\, B}) \qquad (6)$$

By the consistency of the BME tree length estimation, $l(T, D) = l(T) = \omega(T)$. So, for the proof of the consistency of the BME method it sufficed for [13] to demonstrate that $l(W, D) > l(T, D)$ for all $W \in \mathcal{T}_n$ with $W \neq T$. By Equation (6), it was enough to prove this inequality holds for any split metric $D^{A \,|\, B}$ of T in place of D. Likewise, for our proof of Lemma 2, we consider the tree $T \in \mathcal{T}_n$ such that $C_1, \ldots, C_p \in T$. Furthermore, we take an edge-weighting ω of T for which $\omega(e) = 0$ if $e \notin C_i$, for all $1 \leq i \leq p$. We will show that if $W \in \mathcal{T}_n$ contains $C_1, \ldots, C_p$ then $l(W, D) = l(T, D)$. Otherwise if $C_i \notin W$ for some $1 \leq i \leq p$, then we show $l(W, D) > l(T, D)$. Both parts proceed by reducing to the case of split metrics $D^{A \,|\, B}$ for T, and drawing upon the results in [13].

Consider $W \in \mathcal{T}_n$ such that $C_1, \ldots, C_p \in W$. Since $C_i \in W, T$ for all $1 \leq i \leq p$, $\Sigma(W) \cap \Sigma(T)$ contains any split $A \mid B$ induced by any edge $e \in C_1, \ldots, C_p$. As shown in [13] (by direct calculations using the definition of the BME branch lengths l), if a split $A \mid B$ is both in $\Sigma(T)$ and $\Sigma(W)$ then $l(W, D^{A \mid B}) = l(T, D^{A \mid B}) = 1$. If $W \neq T$ then there exist some split $A \mid B$ in $\Sigma(T)$ but not in $\Sigma(W)$, and $\omega(A \mid B) = 0$. Thus $l(W, D) = l(T, D)$. Now consider $W \in \mathcal{T}_n$ such that $C_i \notin W$ for some $1 \leq i \leq p$. As above, there exists some split $A \mid B$ in $\Sigma(T)$ and not in $\Sigma(W)$, and moreover $\omega(A \mid B) > 0$. Under these circumstances, the argument in the (remainder of the) proof of Theorem 2 of [13] applies to show $l(W, D^{A \mid B}) > l(T, D^{A \mid B})$, which suffices to complete the proof of Lemma 2.

$\square$

Proof (Proposition 1). Let $\mathbf{a}, \mathbf{b} \in \text{vert}(\mathcal{P})$ and suppose $\mathbf{a} \in \underset{\mathbf{z} \in \text{vert}(\mathcal{P})}{\text{argmax}} \, \mathbf{z} \cdot \mathbf{c}_1 \not\ni \mathbf{b}$.

Thus $\mathbf{a} \cdot \mathbf{c}_1 > \mathbf{b} \cdot \mathbf{c}_1$. Then

$$\mathbf{a} \cdot (\mathbf{c}_1 + \mathbf{c}_2) - \mathbf{b} \cdot (\mathbf{c}_1 + \mathbf{c}_2) = \mathbf{a} \cdot \mathbf{c}_1 - \mathbf{b} \cdot \mathbf{c}_1 + \mathbf{a} \cdot \mathbf{c}_2 - \mathbf{b} \cdot \mathbf{c}_2$$

$$\geq \min_{\substack{\mathbf{x}, \mathbf{y} \in \text{vert}(\mathcal{P}) \\ \mathbf{x} \in \text{argmax}_{\mathbf{z} \in \mathcal{P}} \, \mathbf{c}_1 \cdot \mathbf{z} \\ \mathbf{c}_1 \cdot \mathbf{x} \neq \mathbf{c}_1 \cdot \mathbf{y}}} \mathbf{c}_1 \cdot \mathbf{x} - \mathbf{c}_1 \cdot \mathbf{y} + \mathbf{a} \cdot \mathbf{c}_2 - \mathbf{b} \cdot \mathbf{c}_2 > 0,$$

since

$$\min_{\substack{\mathbf{x}, \mathbf{y} \in \text{vert}(\mathcal{P}) \\ \mathbf{x} \in \text{argmax}_{\mathbf{z} \in \mathcal{P}} \, \mathbf{c}_1 \cdot \mathbf{z} \\ \mathbf{c}_1 \cdot \mathbf{x} \neq \mathbf{c}_1 \cdot \mathbf{y}}} \mathbf{c}_1 \cdot \mathbf{x} - \mathbf{c}_1 \cdot \mathbf{y} > \max_{\mathbf{x}, \mathbf{y} \in \text{vert}(\mathcal{P})} |\mathbf{c}_2 \cdot \mathbf{x} - \mathbf{c}_2 \cdot \mathbf{y}|.$$

Thus $\mathbf{b} \notin \underset{\mathbf{z} \in \text{vert}(\mathcal{P})}{\text{argmax}} \, (\mathbf{c}_1 + \mathbf{c}_2) \cdot \mathbf{z}$ and therefore

$$\underset{\mathbf{z} \in \text{vert}(\mathcal{P})}{\text{argmax}} \, (\mathbf{c}_1 + \mathbf{c}_2) \cdot \mathbf{z} \subseteq \underset{\mathbf{z} \in \text{vert}(\mathcal{P})}{\text{argmax}} \, \mathbf{c}_1 \cdot \mathbf{z}.$$

$\square$

Proof (Lemma 3). Let $\mathbf{d} \in \mathbb{R}^{\binom{n}{2}}$ be the normal vector of the face F. Let i be a leaf of clade C_1 and j a leaf of clade C_2. Now apply Proposition 1 as follows: There exists $\varepsilon > 0$ sufficiently small such that

$$\min_{\substack{\mathbf{x}, \mathbf{y} \in \text{vert}(\mathcal{P}_n) \\ \mathbf{x} \in \text{argmax}_{\mathbf{z} \in \mathcal{P}_n} \, \mathbf{z} \cdot \mathbf{d} \\ \mathbf{d} \cdot \mathbf{x} \neq \mathbf{d} \cdot \mathbf{y}}} \mathbf{d} \cdot \mathbf{x} - \mathbf{d} \cdot \mathbf{y} > \max_{\mathbf{x}, \mathbf{y} \in \text{vert}(\mathcal{P}_n)} |\varepsilon(-\mathbf{e}_{ij}) \cdot \mathbf{x} - \varepsilon(-\mathbf{e}_{ij}) \cdot \mathbf{y}|.$$

Therefore

$$\underset{T \in \mathcal{T}_n}{\text{argmax}} \, \mathbf{w}^T \cdot (\mathbf{d} - \varepsilon \mathbf{e}_{ij}) = \underset{T \in \text{vert}(F)}{\text{argmax}} \, \mathbf{w}^T \cdot (-\varepsilon \mathbf{e}_{ij})$$

which are precisely all trees contained in $\text{vert}(F)$ such that clades C_1, C_2 are farthest apart. To show there exists an objective corresponding to a face contained in $\text{vert}(F)$ such that clades C_1, C_2 are close as possible, simply change $-\mathbf{e}_{ij}$ to $\mathbf{e}_{ij}$.

$\square$

Proof (Lemma 4). Consider the left-hand side of the inequality in Equation 3 applied to $\mathbf{c}^1, \mathbf{c}^2$ and $\mathcal{P}_n$:

$$\min_{\substack{T'', T' \in \mathcal{P}_n \\ T'' \in \operatorname{argmax}_{T \in \mathcal{T}_n} \mathbf{c}^1 \cdot \mathbf{w}^T \\ \mathbf{c}^1 \cdot \mathbf{w}^{T''} > \mathbf{c}^1 \cdot \mathbf{w}^{T'}}} K \left(\sum_{\{i,j\} \in \operatorname{supp}(\mathbf{c}^1)} (w_{ij}^{T''} - w_{ij}^{T'}) \right). \tag{7}$$

First note that $\frac{1}{2^{n-2}} \leq w_{ij}^T \leq \frac{1}{2}$ for all $T \in \mathcal{T}_n$ and all $\{i, j\}$. Thus,

$$2^{n-2} \sum_{\{i,j\} \in \operatorname{supp}(\mathbf{c}^1)} (w_{ij}^{T''} - w_{ij}^{T'})$$

will be integral and greater than 0. This implies that

$$\sum_{\{i,j\} \in \operatorname{supp}(\mathbf{c}^1)} (w_{ij}^{T''} - w_{ij}^{T'}) \geq \frac{1}{2^{n-2}}.$$

Hence the expression in Equation 7 will be greater than or equal to $\frac{K}{2^{n-2}}$. Using the bounds on w_{ij}^T for all T and $\{i, j\}$, and the triangle inequality,

$$\frac{1}{2} \mathbf{c}^2 \cdot (1, 1, \dots, 1) \geq \max_{T', T'' \in \mathcal{T}_n} |\mathbf{c}_2 \cdot \mathbf{w}^{T''} - \mathbf{c}_2 \cdot \mathbf{w}^{T'}|.$$

Therefore if Equation 4 holds then Proposition 1 holds, completing the proof of Lemma 4.

$\square$

Proof (Lemma 5). Let $\widehat{T} \in \mathcal{T}_n$ and clade $\widehat{C}$ of $\widehat{T}$ be the input of Algorithm 1 with output $\mathbf{c}^1, \mathbf{c}^2, \dots, \mathbf{c}^t$. Moreover, let $K_1, K_2, \dots, K_t$ be the ordered list of K_i used. Let $1 \leq r < t$ and from Step 10 in Algorithm 1 we see that $K_{r+l} < \frac{1}{2^l} \frac{1}{2^{n-2}} \frac{K_r}{\binom{n}{2}}$ for $1 \leq l \leq t - r$.

Then

$$\frac{1}{2}\left(\mathbf{c}^{r+1} + \mathbf{c}^{r+2} + \cdots + \mathbf{c}^t\right) \cdot (1, 1, \ldots, 1)$$

$$=\frac{1}{2}\left(\sum_{\{i,j\}\in\mathrm{supp}(\mathbf{c}^{r+1})} c_{i,j}^{r+1} + \sum_{\{i,j\}\in\mathrm{supp}(\mathbf{c}^{r+2})} c_{i,j}^{r+2} + \cdots + \sum_{\{i,j\}\in\mathrm{supp}(\mathbf{c}^t)} c_{i,j}^t\right)$$

$$=\frac{1}{2}\left(\sum_{\{i,j\}\in\mathrm{supp}(\mathbf{c}^{r+1})} \frac{K_{r+1}}{\binom{n}{2}} + \sum_{\{i,j\}\in\mathrm{supp}(\mathbf{c}^{r+2})} \frac{K_{r+2}}{\binom{n}{2}} + \cdots + \sum_{\{i,j\}\in\mathrm{supp}(\mathbf{c}^t)} \frac{K_t}{\binom{n}{2}}\right)$$

$$<\frac{1}{2}\left(K_{r+1} + \cdots + K_t\right)$$

$$<\frac{1}{2}\left(\frac{1}{2}\frac{1}{2^{n-2}}\frac{K_r}{\binom{n}{2}} + \frac{1}{2^2}\frac{1}{2^{n-2}}\frac{K_r}{\binom{n}{2}} + \cdots + \frac{1}{2^{t-r}}\frac{1}{2^{n-2}}\frac{K_r}{\binom{n}{2}}\right)$$

$$=\frac{1}{2}\frac{1}{2^{n-2}}\frac{K_r}{\binom{n}{2}}\left(\frac{1}{2} + \frac{1}{2^2} + \cdots + \frac{1}{2^{t-r}}\right) < \frac{K_r}{\binom{n}{2}2^{n-2}} = \frac{c_{ij}^r}{2^{n-2}}$$

for $\{i,j\} \in \mathrm{supp}(\mathbf{c}^r)$. Thus $(\mathbf{c}^r, \mathbf{c}^{r+1}+\cdots+\mathbf{c}^t, \mathcal{P}_n)$ satisfies the dominance condition for $1 \le r < t$ and Lemma 4 applies. Therefore $\mathrm{argmax}_{T\in\mathcal{T}_n}(\mathbf{c}^{r+1}+\cdots+\mathbf{c}^t)\cdot \mathbf{w}^T \subseteq \mathrm{argmax}_{T\in\mathcal{T}}\mathbf{c}^r \cdot \mathbf{w}^T$. Altogether this implies that $\mathrm{argmax}_{T\in\mathcal{T}_n}(\mathbf{c}^1 + \cdots + \mathbf{c}^t) \cdot \mathbf{w}^T$ is the set of trees where, and in this order, $\mathbf{c}^1 \cdot \mathbf{w}^T$ is maximized, $\mathbf{c}^2 \cdot \mathbf{w}^T$ is maximized, ..., $\mathbf{c}^t \cdot \mathbf{w}^T$ is maximized. But this recursive linear optimization of $\mathbf{c}^1, \ldots, \mathbf{c}^t$ over $\mathcal{P}_n$ precisely forces the amalgamation of cherries determined in Algorithm 1.

$\square$

Proof (Lemma 6).
Suppose not. That is, for some $1 \le i < j \le t$ and some $1 \le k \le l \le n$, assume $c_{kl}^i > 0$ and $c_{kl}^j > 0$. Since $i < j$ this implies leaves k and l are contained in two separate leaves of T_i in Algorithm 1. Moreover since $c_{kl}^i > 0$, this implies the leaves of T_i that contained k and l were amalgamated, giving T_{i+1}. Thus, leaves k and l will never appear in separate leaves of T_r for any $r > i$. But, $c_{kl}^j > 0$, implying k and l appear in separate leaves of T_j, a contradiction.

$\square$

Proof (Lemma 8). Let $\mathbf{c}^1, \mathbf{c}^2 \in \mathbb{R}_+^{\binom{n}{2}}$ where $|\mathrm{supp}(\mathbf{c}^1)| = 1$, and $(\mathbf{c}^1, \mathbf{c}^2, \mathcal{P})$ satisfies the dominance condition (Equation 4). Further, let $\mathbf{c} = \mathbf{c}^1 + \mathbf{c}^2$, $\{p, q\} = \mathrm{supp}(\mathbf{c}^1)$, and $Q_{-\mathbf{c}}(i, j)$ be the Q-criteria calculated from the dissimilarity map $-\mathbf{c}$. If $n = 4$, and p, q, r, s are the leaves, then we see directly that $Q_{-\mathbf{c}}(p, q) = Q_{-\mathbf{c}}(r, s)$. Moreover $c_{p,q}^1$ appears in $Q_{-\mathbf{c}}(p, r), Q_{-\mathbf{c}}(q, s), Q_{-\mathbf{c}}(p, s), Q_{-\mathbf{c}}(q, r)$, and not in $Q_{-\mathbf{c}}(p, q)$ and $Q_{-\mathbf{c}}(r, s)$. The dominance condition implies $Q_{-\mathbf{c}}(p, q) = Q_{-\mathbf{c}}(r, s) < \min\left(Q_{-\mathbf{c}}(p, r), Q_{-\mathbf{c}}(q, s), Q_{-\mathbf{c}}(p, s), Q_{-\mathbf{c}}(q, r)\right)$.

Now consider $n > 4$. Since $(\mathbf{c}^1, \mathbf{c}^2, \mathcal{P})$ satisfies the dominance condition, it follows that

$$\frac{c_{p,q}^1}{2^{n-2}} = \frac{c_{p,q}}{2^{n-2}} > \frac{1}{2}\left(\sum_{1\leq i<j\leq n} c_{i,j}^2\right) = \frac{1}{2}\left(\sum_{\{i,j\}\neq\{p,q\}} c_{i,j}\right) \qquad \Rightarrow$$

$$\frac{1}{2}c_{p,q} > \sum_{\{i,j\}\neq\{p,q\}} c_{i,j} \qquad \Leftrightarrow$$

$$-\frac{1}{2}c_{p,q} > -c_{p,q} + \sum_{\{i,j\}\neq\{p,q\}} c_{i,j}.$$

This implies

$$Q_{-\mathbf{c}}(p,q) = -(n-4)c_{p,q} + \sum_{k\neq q} c_{p,k} + \sum_{k\neq p} c_{k,q} < -(n-5)c_{p,q} - \frac{1}{2}c_{p,q}.$$

Furthermore, $\frac{1}{2}c_{p,q} > c_{i,j}$ for all $\{i,j\} \neq \{p,q\}$, since the dominance condition is satisfied. Finally

$$Q_{-\mathbf{c}}(p,q) < -(n-5)c_{p,q} - \frac{1}{2}c_{p,q} < -(n-5)c_{i,j} - c_{i,j} = -(n-4)c_{i,j} \leq Q_{-\mathbf{c}}(i,j).$$

$\square$